

PB90-140716

Environmental Software at the U.S. Environmental Protection
Agency's Center for Exposure Assessment Modeling

(U.S.) Environmental Research Lab., Athens, GA

1989



U.S. Department of Commerce
National Technical Information Service

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TECHNICAL REPORT DATA <i>(Please read Instructions on the reverse before completing)</i>		
1. REPORT NO. EPA/600/J-89/191	2.	3. RE PB90-140716
4. TITLE AND SUBTITLE ENVIRONMENTAL SOFTWARE AT THE U.S. ENVIRONMENTAL PROTECTION AGENCY'S CENTER FOR EXPOSURE ASSESSMENT MODELING		5. REPORT DATE
		6. PERFORMING ORGANIZATION CODE
7. AUTHOR(S) Robert B. Ambrose, Jr. and Thomas O. Barnwell, Jr.		8. PERFORMING ORGANIZATION REPORT NO.
9. PERFORMING ORGANIZATION NAME AND ADDRESS Environemntal Research Laboratory U.S. Environmental Protection Agency Athens GA 30613		10. PROGRAM ELEMENT NO. ABWD1A
		11. CONTRACT/GRANT NO.
12. SPONSORING AGENCY NAME AND ADDRESS Environmental Research Laboratory - Athens, GA Office of Research and Development U.S. Environmental Protection Agency Athens GA 30613		13. TYPE OF REPORT AND PERIOD COVERED
		14. SPONSORING AGENCY CODE EPA/600/01
15. SUPPLEMENTARY NOTES Environmental Software 492):76-93, June 1989		
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17. KEY WORDS AND DOCUMENT ANALYSIS		
a. DESCRIPTORS	b. IDENTIFIERS/OPEN ENDED TERMS	c. COSATI Field/Group
REPRODUCED BY U.S. DEPARTMENT OF COMMERCE NATIONAL TECHNICAL INFORMATION SERVICE SPRINGFIELD, VA 22161		
18. DISTRIBUTION STATEMENT RELEASE TO PUBLIC	19. SECURITY CLASS (This Report) UNCLASSIFIED	21. NO. OF PAGES 19
	20. SECURITY CLASS (This page) UNCLASSIFIED	22. PRICE

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ABSTRACT

The Center for Exposure Assessment Modeling (CEAM) was established to meet the scientific and technical exposure assessment needs of the United States Environmental Protection Agency's (EPA) Program and Regional Offices and the various state environmental agencies. To support environmental risk-based decisions concerning protection of air, water, and soil, CEAM provides proven predictive exposure assessment techniques for aquatic, atmospheric, terrestrial, and multimedia pathways for organic chemicals and metals. A wide range of analysis techniques is provided, ranging from simple desk-top techniques suitable for screening analysis through computerized steady-state models to sophisticated, state-of-the-art continuous simulation models. This paper reviews the capabilities of 12 environmental simulation models for urban and rural nonpoint sources, conventional and toxic pollution of streams, lakes and estuaries, tidal hydrodynamics, geochemical equilibrium, and aquatic food chain bioaccumulation.

SOFTWARE AVAILABILITY

CEAM maintains a distribution center for continually updated models (codes and documentation) and databases for users. All computer code distributed by CEAM is considered to be in the public domain and is freely available to users. Persons interested in obtaining the software described in this article should send their requests to the Model Support Section at the authors' address. Requests for PC versions of the software should be accompanied by the proper number of diskettes (see Table I).

Key Words: CEAM, EPA, pollution, multimedia, risk, exposure.

INTRODUCTION

The Center for Exposure Assessment Modeling (CEAM) was established in July 1987 to meet the scientific and technical exposure assessment needs of the United States Environmental Protection Agency's Program and Regional Offices and the States. To support the Agency and professional community in environmental risk-based decisions concerning protection of air, water, and soil, CEAM is working to expand the applications expertise for quantitatively assessing pollutant exposure as part of human and ecological risk assessments. Toward this goal, CEAM provides proven predictive exposure assessment techniques for aquatic, atmospheric, terrestrial, and multimedia pathways for organic chemicals and

metals. CEAM maintains a distribution center for continually updated models (codes and documentation) and databases for users. Qualified users are offered training in courses that feature instructors from EPA and other experts from state government, academia, and the consulting community.

MODEL SUPPORT AND DISTRIBUTION

The modeling packages currently available through the Center were selected from many candidate models by experienced users in EPA regulatory and regional offices and by the Center staff. Selection criteria included model utility and effectiveness, availability of adequate documentation, degree of acceptance and

Paper accepted 24 February 1989

application by users, and the Center staff's experience with the model. A wide selection of analysis techniques is provided, ranging from simple desk-top techniques for screening analysis through computerized steady-state models to sophisticated, state-of-the-art continuous simulation models. Personal computer versions of these computer programs are designed for the PC DOS operating system on the IBM PC XT/AT/PS2 family of microcomputers and compatible systems. The models generally require 640 kB RAM and a 10 MB hard disk for operation. A math coprocessor is highly desirable, but not required except for HSPF.

In response to requests for software, the Center provides a copy of the model documentation and computer code on either a 9-track magnetic tape or, when appropriate, on user-supplied diskettes for IBM-PC compatible personal computers. The programs are written in standard FORTRAN 77 and are maintained for both the IBM PC-compatible and the DEC/VAX with VMS operating system. Executable code is available for the MS/DOS environment. Source code only is available for the VAX environment. These programs have been installed on a wide range of computers world-wide with, at most, minor modifications.

In addition to distribution, the Center also functions as a clearinghouse for correcting code and routine errors or other problems that are discovered as the models are applied. This vital information exchange function helps users obtain correct computations when applying a model developed for one purpose to a new and different problem. New software releases periodically document code updates and corrections to known problems. Model maintenance activities focus on overcoming problems in the use of models; further development, refinement, and extension of these models is a separate research and development activity.

The Center periodically distributes, free of charge, a newsletter to model users and developers. The newsletter provides helpful hints to model users and communicates information on scheduled workshops, model improvements and developments, the availability of technical documents, and planned meetings and conferences.

CEAM operates an Electronic Bulletin Board System (BBS) to meet the increasing demand for exposure assessment models supported by the Center. It allows efficient communication between users with modem-equipped computers and CEAM support staff as well as immediate acquisition of models by those under extreme time pressure. The services presently offered are: 1. downloading of CEAM supported models; 2. uploading of user input data sets for staff review and problem solving; 3. a bulletin area listing current CEAM activities and events, such as training courses, helpful hints about the models, and model documen-

tation; and 4. a message area for discussion of computer modeling problems and enhancements. To access the CEAM BBS, a user must call 404/546-3402 or FTS 250-3402 and follow the interactive prompts. The communications parameters are 9600/2400/1200 baud, no parity, 8 data bits, and 1 stop bit.

CURRENTLY DISTRIBUTED MODELS

The Center currently distributes 12 simulation models. These can be applied to urban runoff (SWMM4, HSPF9), leaching and runoff from soils (PRZM, HSPF9), conventional pollution of streams (QUAL2E, HSPF9, WASP4), toxic pollution of streams (HSPF9, WASP4, EXAMS2, DYNTOX, SARAH2), toxic pollution of lakes and estuaries (WASP4, EXAMS2), conventional pollution of lakes and estuaries (WASP4), tidal hydrodynamics (DYNHYD4), geochemical equilibrium (MINTEQA2), and aquatic food chain bioaccumulation (FGETS, WASP Food Chain Model). The remainder of this paper will summarize these simulation models. The current version number and diskette requirements for PC versions of these models are given in Table I.

Table I - Diskette Requirements for PC Versions of CEAM Models

Model Name	Version Number	Number of 5.25" Disks	Number of 3.5" Disks
DYNTOX	1.0	3	N/A
EXAMSII	2.92	4	N/A
HSPF	9.01	5	2
MINTEQA2/PRODEF	2.01	3	1
PRZM	2.00	2	N/A
QUAL2E-UNCAS	3.00	4	N/A
SWMM4	4.04	4	1
WASP4/TOXI/EUTRO/ DYNHYD4	4.14	3	1
GCSOLAR	1.10	1	N/A
FGETS	1.00	1	N/A
SARAH2	1.00	1	N/A
FCM2	2.00	1	N/A

N/A = Not Available

In addition, GCSOLAR and LC50 are distributed to aid in data analysis for environmental problems. Three new models are being tested and will be distributed in the next year. RUSTIC will simulate unsaturated and saturated transport of pollutants in ground water. MULTIMED will address multimedia exposure from hazardous waste sites. TEEAM will simulate terrestrial exposure and food chain accumulation.

STORM WATER MANAGEMENT MODEL

The Storm Water Management Model (SWMM) was originally developed between 1969 and 1971 and was the first comprehensive model of its type for urban runoff analysis, although it has certainly not remained the only one. Maintenance and improvements to SWMM led to Version 2 in 1975, Version 3 in 1981 and now Version 4 [1]. Version 4 of SWMM is the latest edition of this comprehensive computer model for analysis of quantity and quality problems associated with urban runoff.

Both single-event and continuous simulation may be performed on catchments having storm sewers, combined sewers and natural drainage, for prediction of flows, stages and pollutant concentration. The EXTRAN Block solves the complete dynamic flow routing equations (St. Venant equations) for accurate simulation of backwater, looped connections, surcharging, and pressure flow. Using SWMM, the modeler can simulate all aspects of the urban hydrologic and quality cycles, including rainfall, snowmelt, surface and subsurface runoff, flow routing through the drainage network, storage and treatment. Statistical analyses may be performed on long-term precipitation data and on output from continuous simulation.

The model may be used for both planning and design. The planning mode is used for an overall assessment of the urban runoff problem and proposed abatement options. This mode is typified by continuous simulation for several years using long-term precipitation data. Catchment schematization is usually "coarse" in keeping with the planning level of analysis. The Statistics Block may be used for frequency analysis of the long-term output time series of hydrographs and pollutographs and for identification of individual hydrologic events that may be of special interest. A design-level, event simulation also may be run using a detailed catchment schematization and shorter time steps for precipitation input.

Although the historical basis of the model was for analysis of urban runoff quality problems, the model often is used for pure drainage, hydrologic and hydraulic analysis. The EXTRAN Block has proven especially valuable for sophisticated hydraulic analysis of urban drainage networks.

User Requirements

The model is designed for use by engineers and scientists experienced in urban hydrological and water quality processes. Although the user's manuals explain most computational algorithms, an engineering background is necessary to appreciate most methods being used and to verify that the model results are reasonable.

SWMM Version 4 is principally microcomputer based (IBM PC compatible), although the Fortran code may be compiled on any machine. Execution times are on the order of a few to several minutes for most jobs. Simulation of large areas with many subcatchments and/or channels for many time steps, however, can require several hours on a micro-computer.

Data Requirements

Depending upon the simulation objective, input data requirements can be minimal to extensive. For simulation of a complete drainage network, data collection can be accomplished within a few days, but reducing the data for input to the model may take up to 3 person-weeks for a large area (eg., greater than about 2000 acres). For an EXTRAN simulation of sewer hydraulics, expensive and time consuming field verification of sewer invert elevations often is required. On an optimistic note, however, most data reduction--tabulation of slopes, lengths and diameters--is straightforward.

Calibration data are measured hydrographs and pollutographs for use in establishing values of input parameters for which *a priori* estimates are insufficient. It is often possible to obtain good agreement between predicted and measured hydrographs with little calibration effort. This is not true for quality simulation for which calibration data are essential to obtain credible simulations of pollutographs. Without such measured concentrations and loads, SWMM quality simulation is at best only suited for relative comparisons between control strategies and should not be relied upon for prediction of absolute magnitudes of concentrations and loads. No firm numbers can be given for the required amount of calibration and verification events, but six of each should provide a robust calibration and verification.

When Should SWMM Be Used?

SWMM is a large, relatively sophisticated hydrologic, hydraulic and water quality simulation program. It is not appropriate for all applications or for all personnel, and alternative hydrologic models exist. A large body of literature on theory and case studies is available for SWMM. A bibliography of SWMM-related literature is available [2].

SWMM is certainly formidable both in terms of its size and capabilities. Who, then, should use SWMM and for what purposes? Some criteria for usage are given below:

1. The engineer must be knowledgeable of the modeling techniques (e.g., non-linear reservoirs, kinematic waves, St. Venant equations, buildup-washoff equations) and is assumed to be familiar

with the problem to be solved and with customary techniques for handling it. A clear problem definition is a prerequisite to any solution methodology.

2. By virtue of the problem size (e.g., sewer system with hundreds of pipes) or complexity (e.g., hydraulic controls, backwater), a sophisticated model must be used.
3. Quality must be simulated. Although other models also simulate quality, SWMM is perhaps the most flexible. Of course, SWMM often is applied just to quantity problems.

Users more familiar with an adequate alternative methodology are probably better advised to remain with that methodology. In the final analysis, the engineer/analyst is responsible for the decisions made using any technique of analysis; the technique or model is only a tool that must be clearly understood by those using it.

HYDROLOGIC SIMULATION PROGRAM - FORTRAN

Hydrological Simulation Program - FORTRAN (HSPF), [3], [4] is a comprehensive package for simulation of watershed hydrology and water quality for both conventional and toxic organic pollutants. HSPF incorporates the watershed-scale ARM and NPS models into a basin-scale analysis framework that includes fate and transport in one-dimensional stream channels. It is the only comprehensive model of watershed hydrology and water quality that allows the integrated simulation of land and soil contaminant runoff processes with in-stream hydraulic and sediment-chemical interactions.

The result of this simulation is a time history of the runoff flow rate, sediment load, and nutrient and pesticide concentrations, along with a time history of water quantity and quality at any point in a watershed. HSPF simulates three sediment types (sand, silt, and clay) in addition to a single organic chemical and transformation products of that chemical. The transfer and reaction processes included are hydrolysis, oxidation, photolysis, biodegradation, volatilization, and sorption. Sorption is modeled as a first-order kinetic process in which the user must specify a desorption rate and an equilibrium partition coefficient for each of the three solids types. Resuspension and settling of silts and clays (cohesive solids) are defined in terms of shear stress at the sediment-water interface. The capacity of the system to transport sand at a particular flow is calculated and resuspension or settling is defined by the difference between the sand in suspension and the transport capacity. Calibration of the model requires data for

each of the three solids types. Benthic exchange is modeled as sorption/desorption and deposition/scour with surficial benthic sediments. Underlying sediment and pore water are not modeled.

Data Needs/Availability

Data needs for HSPF can be extensive. HSPF is a continuous simulation program and requires continuous data to drive the simulations. As a minimum, continuous rainfall records are required to drive the runoff model and additional records of evapotranspiration, temperature, and solar intensity are desirable. A large number of model parameters can be specified although default values are provided where reasonable values are available. HSPF is a general-purpose program and special attention has been paid to cases where input parameters are omitted. Option flags allow bypassing of whole sections of the program where data are not available.

Output of the Assessment

HSPF produces a time history of the runoff flow rate, sediment load, and nutrient and pesticide concentrations, along with a time history of water quantity and quality at any point in a watershed. Simulation results can be processed through a frequency and duration analysis routine that produces output compatible with conventional toxicological measures (e.g., 96-hour LC50).

Limitations

HSPF assumes that the "Stanford Watershed Model" hydrologic model is appropriate for the area being modeled. Further, the instream model assumes the receiving water body is well-mixed with width and depth and is thus limited to well-mixed rivers and reservoirs. Application of this methodology generally requires a team effort because of its comprehensive nature.

Experience

HSPF and the earlier models from which it was developed have been extensively applied in a wide variety of hydrologic and water quality studies [5], [6], including pesticide runoff model testing [7], aquatic fate and transport model testing [8], [9], analyses of agricultural best management practices [10], [11], and as part of pesticide exposure assessments in surface waters.

An application of HSPF in a screening methodology for pesticide review is described by Donigian et al. [12]. The Stream Transport and Agricultural Runoff for Exposure Assessment Methodology (STREAM) applies the HSPF program to various test watersheds for five major crops in four agricultural

regions in the United States, defines a "representative" watershed based on regional conditions and an extrapolation of the calibration for the test watershed, and performs a sensitivity analysis on key pesticide parameters to generate cumulative frequency distributions of pesticide loads and concentrations in each region. The resulting methodology requires the user to evaluate only the crops and regions of interest, the pesticide application rate, and three pesticide parameters -- the partition coefficient, the soil/sediment decay rate, and the solution decay rate.

Validation/Review

The program has been validated with both field data and model experiments and has been reviewed by independent experts.

PESTICIDE ROOT ZONE MODEL

Pesticide Root Zone Model (PRZM) [13], [14], is a dynamic compartment model that simulates the vertical movement of pesticides and other organic chemicals in unsaturated soil, both within and below the plant root zone. PRZM allows the user to perform dynamic simulations of potentially toxic chemicals that are applied to the soil or to plant foliage. Dynamic simulations allow the consideration of pulse loads, the prediction of peak events, and the estimation of time-varying mass emission or concentration profiles. Simulations may extend to the water table using generally available input data that are reasonable in spatial and temporal requirements.

The model consists of hydrology and chemical transport components that simulate runoff, erosion, plant uptake, leaching, decay, foliar wash off, and volatilization (implicitly) of a pesticide. Predictions can be made daily, monthly, or annually. PRZM has a separate interactive processing module to develop and update parameter files for calibration, verification, and production runs.

Variables and Processes

PRZM has two components: hydrology and chemical transport. The hydrology component for calculating runoff and erosion is based on the Soil Conservation Service curve number technique and the universal soil loss equation. Evapotranspiration is divided among evaporation from crop interception, evaporation from soil, and transpiration from the crop. Water movement is simulated by the use of generalized soil terms including field capacity, wilting point, and saturation. Drainage from loose, porous and tighter compact soils is simulated. To produce soil water and solid phase concentrations, the chemical transport component calculates pesticide uptake by plants,

surface runoff, erosion, decay, vertical movement, foliar loss, dispersion, and retardation. A finite difference numerical solution, using a backwards - difference implicit scheme, is employed.

Data Needs

PRZM requires information on two major components -- hydrology and chemical transport. Daily rainfall and pan evaporation data are required to drive the hydrology simulation. Generalized soil terms including field capacity, wilting point and saturation must be specified. The chemical transport component of PRZM requires information on pesticide partitioning and degradation rates. The users manual provides detailed guidance on parameter estimation and model operation as well as an example application.

Output of the Assessment

The output of a PRZM assessment is a time series of chemical leachate mass and concentration leaving the root zone and entering the water table. This represents a measure of the potential for leaching of the chemical given daily changes in precipitation, evapotranspiration, cropping practices, land management activities, and application timing.

Limitations

The model is limited to estimation of the vertical movement of contaminants. Water is assumed to drain through the soil layers only on days when rainfall events occur.

Experience

The program has been used in a wide range of regulatory applications for the U. S. Environmental Protection Agency. Specific applications can be reviewed in the references [13], [15], [16], [17]. A screening methodology based on prepared scenarios using PRZM has seen wide use in evaluation of pesticide leaching potential [18]. The program has been validated with both field data and model experiments and has been reviewed by independent experts.

STREAM WATER QUALITY MODEL QUAL2E

The Enhanced Stream Water Quality Model QUAL2E and QUAL2E-UNCAS [19] permits simulation of several water quality constituents in a branching stream system using a finite difference solution to the one-dimensional advective-dispersive mass transport and reaction equation. The conceptual representation of a stream used in the QUAL2E formulation is a stream reach that has been divided into a number of subreaches or computational elements equivalent to finite differences. For each computational element, a hydrologic balance in terms of flow (Q), a heat balance in terms of temperature (T), and a materials balance in terms of concentration (C) is written. Both advective and dispersive transport are considered in the materials balance. Mass can be gained or lost from the element by transport processes, external sources and sinks (e.g., waste discharges or withdrawals) or by internal sources and sinks (e.g., benthic sources or biological transformations). The equation is solved for the steady-flow, steady state condition in a classical implicit backward difference method. The specific equations and solution technique are described in detail in the QUAL2E computer program documentation.

The QUAL series of computer programs has a long history in water quality management. The foundation upon which the series is built was laid by the Texas Water Development Board (TWDB) in the late 1960s. In the early 1970s, EPA began a program to provide water quality models for major river basins and specified that QUAL-I be used as the basis for developing new, more advanced, basin-specific models. Many versions of the QUAL-II model emerged from this effort. One in particular was further improved in the mid-1970s for the Southeast Michigan Council of Governments (SEMCOG), the areawide wastewater planning agency for the Detroit metropolitan area. Because of its flexibility and thorough documentation, the SEMCOG version of QUAL-II, known as QUAL-II/SEMCOG received widespread use, especially in wasteload allocation studies.

In the late 1970's, the National Council of the Paper Industry for Air and Stream Improvement (NCASI) undertook a thorough review, testing and documentation project covering a variety of water quality models, including QUAL-II/SEMCOG. Changes resulting from this review were incorporated in the program and the model was renamed QUAL-II/NCASI. NCASI and other groups such as the U. S. Geological Survey (USGS) tested the revised program on several intensively sampled rivers across the United States. Recently, the model has seen several European applications in England, Greece, Belgium and Spain. Other applications of QUAL-II range from South America to the Far East, including South Korea, the

People's Republic of China, and Thailand. A number of applications and ongoing work with the QUAL2E model are described by Barnwell et al. [20].

Prototype Representation

Prototype representation in QUAL2E consists of dividing a stream in a network of "Headwaters", "Reaches", and "Junctions." The fundamental reason for subdividing sections of stream into "Reaches" is that QUAL2E assumes that some 26 physical, chemical and biological properties (model input parameters or coefficients) are constant along a "Reach." The question that must be addressed in order to define a "Reach" is what constitutes "significant" change in these model inputs -- "significant" in the sense of their impact on simulation results, not necessarily in the sense of change in the inputs themselves.

Mass transport in the QUAL2E computer program is handled in a relatively simple manner. There seems to be some confusion about QUAL2E's transport capabilities as it is sometimes called a "dynamic" model. However, in all of the computer programs in the QUAL series, there is an explicit assumption of steady flow; the only time-varying forcing functions are the climatologic variables that primarily affect temperature and algal growth. A more proper term for this capability is "diel," indicating variation over a 24-hour period. The forcing function used for estimating transport is the streamflow rate, which, as mentioned above, is assumed to be constant. Stream velocity, cross-sectional area, and depth are computed from streamflow.

One of the most important considerations in determining the assimilative capacity of a stream is its ability to maintain an adequate dissolved oxygen concentration. The QUAL2E computer program includes the major interactions of the nutrient cycles, algal production, benthic and carbonaceous oxygen demand, atmospheric reaeration, and their effect on the dissolved oxygen balance (Figure 1). In addition, the computer program includes a heat balance for the computation of temperature and mass balances for conservative minerals, coliform bacteria, and non-conservative constituents such as radioactive substances. Chlorophyll *a* is modeled as the indicator of planktonic algae biomass in QUAL2E.

As shown in Figure 1, the nitrogen cycle is composed of four compartments: Organic nitrogen, Ammonia nitrogen, Nitrite nitrogen, and Nitrate nitrogen. The phosphorus cycle is similar to, but simpler than, the nitrogen cycle, having only two compartments. Ultimate carbonaceous biochemical oxygen demand (BOD) is modeled as a first-order degradation process in QUAL2E, which also takes into account removal by settling and does not affect the oxygen balance. QUAL2E will convert the traditional

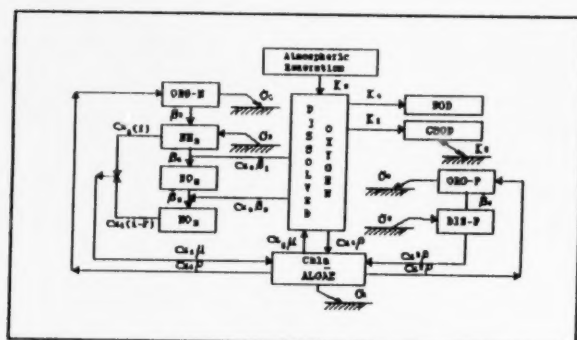


Figure 1 - QUAL2E Constituent Interactions

5-day BOD values to ultimate BOD for internal calculations. The processes discussed above represent the primary internal sinks of dissolved oxygen in the QUAL2E computer program. The major source of dissolved oxygen, in addition to that supplied from algal photosynthesis, is atmospheric reaeration.

Uncertainty Analysis

A major problem faced by the user when working with a complex model such as QUAL2E is model calibration and determination of the most efficient plan for collection of calibration data. This problem can be addressed by application of principles of uncertainty analysis. These strategies have been applied to QUAL2E and the resulting computer program is named QUAL2E-UNCAS. Three uncertainty analysis techniques are employed in QUAL2E-UNCAS: sensitivity analysis, first order error analysis, and monte carlo simulation. The computer program uses pre- and post-processing algorithms to select the input variables and/or parameters to be altered without the user having to manually restructure the input data set and to store and manipulate only the output of interest. The modeler is free to select the important variables and locations in the stream network where uncertainty effects are desired.

User Requirements

In its present state, QUAL2E requires some degree of modeling sophistication and expertise on the part of a user. The user must supply more than 100 individual inputs, some of which require considerable judgment to estimate. The uncertainty analysis procedures incorporated in the computer program serve both to guide the user in the calibration process as well as to provide information about the uncertainty associated with calibrated model.

WATER QUALITY ANALYSIS SIMULATION PROGRAM

Water Quality Analysis Simulation Program, WASP4 [21] is a generalized framework for modeling contaminant fate and transport in surface waters. WASP4 is the latest of a series of WASP programs [22], [23], [24], [25]. Based on the flexible compartment modeling approach, WASP can be applied in one, two, or three dimensions. WASP is designed to permit easy substitution of user-written routines into the program structure. Problems that have been studied using the WASP framework include biochemical oxygen demand and dissolved oxygen dynamics, nutrients and eutrophication, bacterial contamination, and organic chemical and heavy metal contamination.

Two WASP models are provided with WASP4. The toxics WASP model, TOXI4, combines a kinetic structure adapted from EXAMS2 [26] with the WASP4 transport structure and simple sediment balance algorithms to predict dissolved and sorbed chemical concentrations in the bed and overlying waters. The dissolved oxygen/eutrophication WASP model EUTRO4 combines a kinetic structure adapted from the Potomac Eutrophication Model [27] with the WASP4 transport structure to predict DO and phytoplankton dynamics affected by nutrients and organic material.

WASP4 input and output linkages also have been provided to other stand-alone models. Flows and volumes predicted by the link-node hydrodynamic model DYNHYD4 can be read and used by WASP4. Loading files from PRZM and HSPF can be reformatted and read by WASP4. Toxicant concentrations predicted by TOXI4 can be read and used by both the WASP Food Chain Model and the fish bioaccumulation model FGETS.

Prototype Representation

A body of water is represented in WASP as a series of computational elements or segments. Environmental properties and chemical concentrations are modeled as spatially constant within segments. Segment volumes and type (surface water, subsurface water, surface benthic, subsurface benthic) must be specified, along with hydraulic coefficients for riverine networks.

Structurally, the WASP4 program includes six mechanisms for describing transport. These "transport fields" consist of advection and dispersion in the water column; advection and dispersion in the pore water; settling, resuspension, and sedimentation of up to three classes of solids; and evaporation or precipitation. To describe advection within WASP4, each inflow or circulation pattern requires specification of

the fraction routed through relevant water column segments and the time history of the corresponding flow. Dispersion requires specification of cross-sectional areas between model segments, characteristic mixing lengths, and the time history of the corresponding dispersion coefficient.

For each state variable (termed "system" in WASP), the user must specify loads, boundary concentrations, and initial concentrations. The dissolved fractions of each variable also must be specified for each segment. Only dissolved concentrations are transported by pore water and only particulate concentrations are transported by solids.

Each variable is advected and dispersed among water segments, and exchanged with surficial benthic segments by diffusive mixing. Sorbed or particulate fractions may settle through water column segments and deposit to or erode from surficial benthic segments. Within the bed, dissolved variables may migrate downward or upward through percolation and pore water diffusion. Sorbed variables may migrate downward or upward through net sedimentation or erosion.

TOXI4

TOXI4 simulates the transport and transformation of one to three chemicals and one to three types of particulate material. The three chemicals may be independent, such as isomers of PCB, or they may be linked with reaction yields, such as a parent compound-daughter product sequence. Each chemical exists as a neutral compound and up to four ionic species. The neutral and ionic species can exist in five phases: dissolved, sorbed to dissolved organic carbon (DOC), and sorbed to each of the up to three types of solids. Local equilibrium is assumed so that the distribution of the chemical between each of the species and phases is defined by distribution or partition coefficients. The model, then, is composed of up to six systems, three chemical and three solids, for which the general WASP4 mass balance equation is solved.

In an aquatic environment a toxic chemical may be transferred between phases and may be degraded by any of a number of chemical and biological processes. Transfer processes defined in the model include sorption, ionization, and volatilization. Transformation processes defined include biodegradation, hydrolysis, photolysis and chemical oxidation. Sorption and ionization are treated as equilibrium reactions. All other processes are described by rate equations. Rate equations may be quantified either by first-order constants or by second-order chemical specific constants and environment-specific parameters that may vary in space and time.

TOXI4 treats sediment as a conservative constituent that is advected and dispersed among water segments, that settles to and erodes from benthic segments, and that moves between benthic segments through net sedimentation or erosion. Settling, deposition, resuspension, and burial velocities are not calculated, but must be input by the user.

Data Needs

The environmental and chemical database for TOXI4 simulations is standard for chemical-specific models (see EXAMS, below). Those data required for a particular simulation depend upon which transformation processes are important. Up to 12 spatially-variable environmental parameters in TOXI4, such as pH and light extinction, may be specified as needed. The compounds' chemical properties control what transformation processes are important in a particular environment. Molecular weight and solubility should always be specified. Other influential chemical properties should be specified as needed. Up to 17 time variable functions in TOXI4 can be used to study diurnal or seasonal effects on pollutant behavior. Some of these time functions are multiplied by spatially variable parameters within TOXI4 to produce time- and spatially-variable environmental conditions. If no time variability is required, the time functions may be omitted.

Although the amount and variety of data potentially used by TOXI4 is large, data requirements for any particular simulation can be quite small. Usually only sorption and one or two transformation processes will significantly affect a particular chemical. To simulate the transport of many soluble compounds in the water column, even sorption can often be disregarded. Indeed, for empirical studies, all chemical constants, time functions, and environmental parameters can be ignored except a user-specified transformation rate constant and the partition coefficient.

Output of the Assessment

TOXI4 calculates time variable sediment and chemical concentrations for every segment in a specialized network that may include surface water, underlying water, surface bed, and underlying bed. Chemical concentrations are reported for the dissolved, sediment sorbed, and DOC sorbed phases, and as neutral and ionic concentrations. In addition, calculated transformation and transfer rates are reported.

Limitations

Some limitations should be kept in mind when applying TOXI4. First, chemical concentrations should be near trace levels, i.e., below half the solubility or 10^{-5} molar. At higher concentrations,

the assumptions of linear partitioning and transformation begin to break down. Chemical density may become important, particularly near the source, such as in a spill. Large concentrations can affect key environmental characteristics, such as pH or bacterial populations, thus altering transformation rates. TOX14 does not include such feedback phenomena.

EUTRO4

EUTRO4 simulates the transport and transformation of up to eight state variables in the water column and sediment bed, including dissolved oxygen, carbonaceous biochemical oxygen demand, phytoplankton carbon and chlorophyll a, ammonia, nitrate, organic nitrogen, organic phosphorus, and orthophosphate. EUTRO4 can be used to simulate any or all of these variables and the interactions between them. Each variable may exist in both dissolved and particulate phases, as specified by the user for each segment. Solids transport fields describing settling and resuspension of organic solids, phytoplankton solids, and inorganic solids may be specified. The particulate concentration of each variable will be transported by the appropriate solids field.

By bypassing variables and computations, EUTRO4 can be operated at various levels of complexity. The simplest level, equivalent to an enhanced "Streeter-Phelps" equation, includes ultimate BOD, DO, and sediment oxygen demand (SOD). The reaeration rate constant is specified. The next level divides BOD into carbonaceous (CBOD) and nitrogenous (NBOD) fractions. Level 3 is a linear DO balance influenced by photosynthesis and respiration of user-specified phytoplankton and nitrification of ammonia to nitrate, as well as CBOD and SOD. The reaeration rate is computed from velocity, depth, and wind speed. Level 4 adds the phosphorus cycle and simulates phytoplankton dynamics subject to Michaelis-Menten nutrient limitation and light limitation. Level 5 adds benthic interactions explicitly.

Data Needs

The environmental and chemical database for EUTRO4 is standard for DO and eutrophication simulations. Those data required for a particular simulation depend upon which level of complexity is chosen. Up to 16 spatially variable environmental parameters and 60 rate constants in EUTRO4 may be specified as needed. Up to 14 time variable functions in EUTRO4 can be used to study diurnal or seasonal effects on pollutant behavior. Some of these time functions are multiplied by spatially variable parameters within EUTRO4 to produce time- and spatially-variable environmental conditions. If no time variability is required, the time functions may be omitted.

Output of the Assessment

EUTRO4 calculates time variable concentrations for every segment in a specialized network that may include surface water, underlying water, surface bed, and underlying bed. Variable concentrations are reported at user-specified intervals, along with calculated transformation and transfer rates.

Experience

Various WASP models have been used in a wide range of regulatory applications for the U. S. Environmental Protection Agency. Many applications of WASP have been published, including [28], [29], [9], [8]. Some applications have been validated with field data, or verified by model experiments and reviewed by independent experts. Applying WASP4 requires both modeling sophistication and appropriate scientific and engineering judgment.

TIDAL HYDRODYNAMIC MODEL

DYNHYD4 [21] is a simple link-node hydrodynamic model capable of handling variable tidal cycles, wind, and unsteady inflows. This program is an enhancement of the Potomac Estuary hydrodynamic model DYNHYD2 [30] which was a component of the Dynamic Estuary Model [31]. DYNHYD4 solves the one-dimensional equations of continuity and momentum for a branching or channel-junction (link-node) computational network. Driven by variable upstream flows and downstream heads, simulations typically proceed at 1- to 5-minute intervals. The resulting unsteady flows and volumes are averaged over larger time intervals and stored for later use by the WASP4 water quality program.

Variables and Processes

DYNHYD4 solves one-dimensional equations describing the propagation of a long wave through a shallow water system while conserving both momentum (energy) and volume (mass). The equation of motion, based on the conservation of momentum, predicts water velocities and flows. The equation of continuity, based on the conservation of volume, predicts water heights (heads) and volumes. The equation of motion includes terms accounting for local inertia, convective inertia, gravitational acceleration, frictional resistance, and wind stress along the channel axis. The equations are solved by a two step Runge-Kutta procedure.

Data Needs

Data requirements include description of the physical geometry and the forcing functions. For junction elements, initial surface elevation, surface area, and bottom elevation must be given. For channel elements, length, width, hydraulic radius, channel orientation, initial velocity, and Manning's roughness coefficient are required. Significant inflows and outflows can be specified as constant or time-variable. Seaward boundary elevations can be described by describing an average repetitive tidal function or by specifying the high and low tidal heights versus time for multiple tidal cycles. Wind speed and direction can be given as a function of time.

Output of the Assessment

DYNHYD4 calculates time variable channel flows and junction volumes throughout a specialized link-node network. These are summarized for examination, and stored in a file for later import to the WASP4 water quality model.

Limitations

DYNHYD4 assumes that flow is predominantly one-dimensional, that Coriolis and other accelerations normal to the direction of flow are negligible, that channels can be adequately represented by a constant top width with a variable hydraulic depth (i.e., "rectangular"), that the wave length is significantly greater than the depth, and that bottom slopes are moderate. Although no strict criteria are available for the latter two assumptions, most natural flow conditions in large rivers and estuaries would be acceptable.

Experience

Various versions of DYNHYD have been applied to several estuaries as part of waste load allocation studies. These have been calibrated and validated with field data. Applying DYNHYD4 requires both modeling sophistication and engineering judgment.

EXPOSURE ANALYSIS MODELING SYSTEM

EXAMS is an interactive modeling system that allows a user to specify and store the properties of chemicals and ecosystems, modify either via simple commands, and conduct rapid evaluations and error analyses of the probable aquatic fate of synthetic organic chemicals [26]. EXAMS combines the loadings, transport, and transformations of a chemical into a set of differential equations using the law of conservation of mass as an accounting principle. It accounts for all the chemical mass entering and leaving a

system as the algebraic sum of external loadings, transport processes that export the compound from the system, and transformation processes within the system that convert the chemical to daughter products. The program produces output tables and simple graphics describing chemical exposure, fate, and persistence.

Prototype Representation

EXAMS is a computer-based system for installing and running chemical simulation studies with models of aquatic ecosystems. EXAMS' environmental models are maintained in a file composed of concise ("canonical") descriptions of aquatic systems. Each waterbody is represented via a set of segments or distinct zones in the system. The program is based on a series of mass balances for the segments that give rise to a single differential equation for each. Working from the transport and transformation process equations, EXAMS compiles an equation for the net rate of change of chemical concentration in each segment. The resulting system of differential equations describes the mass balance for the entire system. EXAMS includes a descriptor language that simplifies the specification of system geometry and connectedness.

Variables and Processes

EXAMS includes process models of the physical, chemical, and biological phenomena governing the transport and fate of compounds. Each of the unit process equations used to compute the kinetics of chemicals accounts for the interactions between the chemistry of a compound and the environmental forces that shape its behavior in aquatic systems. This "second-order" or "system-independent" approach lets one study the fundamental chemistry of compounds in the laboratory and then, based on independent studies of the levels of driving forces in aquatic systems, evaluate the probable behavior of the compound in systems that have never been exposed to it. Most of the process equations are based on standard theoretical constructs or accepted empirical relationships. The user can specify reaction pathways for the production of transformation products of concern, whose further fate and transport can then be simultaneously simulated by EXAMS.

EXAMS computes the kinetics of volatilization, as well as transformations attributable to direct photolysis, hydrolysis, biolysis, and oxidation reactions. EXAMS has been designed to accept standard water quality parameters and system characteristics that are commonly measured by limnologists throughout the world, and chemical datasets conventionally measured or required by EPA regulatory procedures.

Data Needs

Although EXAMS allows for the entry of extensive environmental data, derived either from limnological literature or field surveys, the program can be run with a much reduced data set when the chemistry of a compound of interest precludes some of the transformation processes. For example, pH and pOH data can be omitted in the case of neutral organics that are not subject to acid or alkaline hydrolysis. Input parameters include:

1. A set of chemical loadings on each sector of the ecosystem.
2. Molecular weight, solubility, and ionization constants of the compound.
3. Sediment-sorption and biosorption parameters: K_p , K_{oc}/K_{ow} , biomass, benthic water content and bulk density, suspended sediment concentration, sediment organic carbon, and ion exchange capacity.
4. Volatilization parameters: Henry's Law constant or vapor pressure data, wind speeds, and reaeration rates.
5. Photolysis parameters: reaction quantum yield, absorption spectra, stratospheric ozone, cloudiness, relative humidity, dust content and air-mass type, scattering parameters, suspended sediments, chlorophyll, and dissolved organic carbon.
6. Hydrolysis: second-order rate constants and Arrhenius functions for the relevant molecular species; pH, pOH, and temperatures.
7. Oxidation: rate constants, temperatures, surface oxidant concentrations, dissolved organic carbon and oxygen tension.
8. Biotransformation: rate constants, temperatures, bacterial population densities.
9. Parameters defining strength and direction of advective and dispersive transport pathways.
10. System geometry and hydrology: volumes, areas, depths, rainfall, evaporation rates, entering stream and non-point-source flows and sediment loads, and ground water flows.

Output of the Assessment

EXAMS output includes 20 tables summarizing input data and predictions of chemical exposure, fate, and persistence. The exposure summary includes the expected (long-term chronic, 24-hour and 96-hour acute) environmental concentrations due to a user-specified pattern of chemical loadings. The fate

summary gives the distribution of chemical in the system and the relative dominance of each transport and transformation process. Finally, the model describes persistence as the time required for effective purification of the system (via export/transformation processes) once chemical loadings terminate. Printer-plots of longitudinal and vertical concentration profiles, as well as time-based graphics, can be invoked by the user.

Limitations

EXAMS has been designed to evaluate the consequences of longer-term, primarily time-averaged chemical loadings that ultimately result in trace-level contamination of aquatic systems. EXAMS generates a steady-state, average flow field (long-term or monthly) for the ecosystem. The program thus cannot fully evaluate the transient concentrated EECs that arise, for example, from chemical spills. The chemical is assumed not to radically change the environmental variables that drive its transformations. Thus, for example, an organic acid or base is assumed not to change the pH of the system. EXAMS uses linear sorption isotherms, and second-order (rather than Michaelis-Menten-Monod) expressions for biotransformation kinetics. This approach is known to be valid for low concentrations of pollutants; its validity at high concentrations is less certain.

Sorption is treated as a thermodynamic or constitutive property of each segment of the system, that is, sorption/desorption kinetics are assumed to be rapid compared to other processes. The adequacy of this assumption is partially controlled by properties of the chemical and system being evaluated. EXAMS does not simulate the solids with which the chemical interacts. The concentration of solids must be specified for each compartment; the program accounts for sorbed chemical transport based on solids concentrations and specified transport fields. Benthic exchange includes pore water advection, and a bulk exchange based on an empirical volumetric dispersion coefficient.

Experience

The program has been used in a wide range of regulatory applications for the U. S. Environmental Protection Agency. The program has been validated with both field data and model experiments and has been reviewed by independent experts. Three such applications are discussed in [32], [9], and [8].

DYNAMIC TOXICITY MODEL

DYNTOX [33] is a waste load allocation computer program that uses probabilistic dilution techniques [34] to estimate concentrations of toxic substances or fractions of whole effluent toxicity. DYNTOX performs three types of simulations -- continuous, monte carlo, and log normal -- that, based on probabilities, can aid in analyzing the frequency and duration of toxic concentrations from a waste discharge. DYNTOX considers dilution and net first-order loss, but not sorption and benthic exchange. The net loss rate must be determined empirically on a case-by-case basis, and should not be extrapolated to different conditions of flow, temperature, solids, pH, or light.

Data Needs

DYNTOX requires input of flow and concentration information for a stream and a waste source. Each type of simulation requires different types of data. The continuous simulation requires continuous daily records of flow and concentration for both the waste and the dilution flow. The monte carlo method uses a lag-one markov process and requires mean, variance, and lag-one correlation coefficients for the four inputs. The log-normal methodology requires mean and variance for the log-normal distributions of the four inputs. A toxicity measure (e.g., LC_{50}) for the contaminant is required for evaluation of the output.

Output of the Assessment

Output of the assessment is the frequency and duration of daily average contaminant concentration in the receiving water body.

Limitations

DYNTOX considers complete dilution of the effluent in the stream, and so cannot be used for near field analyses. The loss rate of toxicity downstream must be derived from site-specific field measurements, and cannot be extrapolated to different effluents or streams.

Experience

The program has been used in regulatory applications for the U.S. EPA [35]. Specific examples can be reviewed in the methodology's references. The program has been validated with model experiments and has been reviewed by independent experts.

HAZARDOUS WASTE SCREENING MODEL

SARAH2 is a nearfield surface water model that calculates maximum allowable concentrations of hazardous wastes discharged to land disposal or waste water treatment facilities based upon predicted exposure to humans or aquatic life [36]. The program has been used in regulatory applications for the U. S. EPA. Its core equations were developed in support of the Land Disposal Banning Rule published in proposal form in the January 14, 1986, Federal Register.

The surface water contamination pathways analyzed in SARAH2 include ground water leachate from a land disposal facility or lagoon, storm runoff from a land disposal facility or lagoon, and discharge through a waste water treatment facility or lagoon. The human exposure pathways considered include ingestion of treated drinking water and consumption of contaminated fish. Acceptable leachate or treated industrial waste discharge constituent concentrations are estimated by a "back calculation" procedure starting from chemical safety criteria in surface water, drinking water, or fish. "Forward calculations" predict the instream concentrations from leachate or discharge concentrations.

SARAH2 is an interactive, menu-driven computer program with three default data sets that can be rapidly modified. The analytical solutions for contaminant behavior in a catchment or stream near the facility allow rapid, multiple calculations needed for good sensitivity analysis.

Variables and Processes

For steady or batch waste streams, SARAH2 considers the following concentration reductions: dilution and loss during treatment, initial Gaussian mixing at the edge of a stream, lateral and longitudinal diffusion in the mixing zone, sorption, volatilization, hydrolysis, and bioaccumulation in fish. The user must specify appropriate in-stream criteria for protection of the aquatic community, and of humans through consumption of fish and water. The benthic community is not presently considered. Treatment loss is handled empirically. Human exposure pathways considered include ingestion of treated drinking water and consumption of contaminated fish.

Data Needs

SARAH2 includes three predefined data sets that can be rapidly modified. The first data set represents a small, flat watershed containing a large land disposal facility and a slow, shallow stream. The second data set represents a small, moderately steep watershed containing a medium-sized land disposal facility

and a faster, deeper stream. The third set reflects a large, steep watershed containing a large land disposal facility and a fast, shallow stream. All three may contain a steady industrial waste discharge.

Output of the Assessment

Standard output from SARAH2 is the allowable leachate or raw waste concentration for user-defined combinations of loading and exposure scenarios. Seven loading scenarios are defined: steady leaching from a land disposal site, storm runoff from a land disposal site, catastrophic release from a storm detention basin, continuous discharge to a wastewater treatment facility, batch discharge to a wastewater treatment facility, leaching from a waste lagoon, and catastrophic release from a wastewater lagoon. Three exposure scenarios are defined: human exposure through drinking water, human exposure through fish consumption, and toxicity to aquatic organisms. SARAH2 also will calculate the human exposure or aquatic toxicity resulting from specified leachate or raw waste releases.

Limitations

SARAH2 is designed for rapid screening analysis of the potential hazard due to disposal of a waste in a land disposal facility or wastewater treatment facility. It contains a number of assumptions about the environment that should be verified if it is applied to actual cases.

Experience

As a screening model, SARAH2 can be applied without extensive modeling experience. Users should be familiar with the model's assumptions and the regulatory framework. The program has been validated with model experiments and has been reviewed by independent experts.

METALS SPECIATION MODEL

MINTEQA2 is an equilibrium chemical speciation model for dilute aqueous systems [37]. The model is an update of MINTEQ [38], which itself was created from the models MINEQL [39] and WATEQ3 [40]. MINTEQA2 is appropriate for calculating the equilibrium composition of dilute solutions in the laboratory or in natural aquatic systems. It can be used to calculate the mass distribution at equilibrium among dissolved, adsorbed, and solid phases under a variety of conditions. The species distribution within each phase also is calculated.

The aqueous equilibrium composition is obtained by calculating the concentrations of all dissolved

species from an initial guess of the activity of each component and from the known stoichiometry of each component in each reaction with known formation constants. The total dissolved mass for each component implied by the calculated concentration of each species is compared with the known total dissolved mass supplied by the user. For each component, if the calculated total mass does not match the known total mass to within a pre-set tolerance level, the activity guess of each component is adjusted in such a way as to compensate for the mass imbalance and the entire procedure is repeated beginning with re-calculating the concentrations of all dissolved species using the new component activity guesses. This iterative procedure is continued until the mass imbalance for every component is less than the tolerance level. When that condition is met, the system is at equilibrium with respect to dissolved species.

Variables and Processes

There are 91 chemical components currently available in MINTEQA2 and an additional 25 components that are specific to certain of the adsorption sub-models. The chemical components include major ions commonly found in natural aqueous systems (Ca, Fe, S, etc.) as well as 13 trace metals/metalloids of particular interest in environmental problems (Ag, As, Ba, Cd, Cr, Cu, Hg, Ni, Pb, Sb, Se, Tl, and Zn) and other metals. Organic ligands of significant affinity for metal complexing also are included. MINTEQA2 is accompanied by a thermodynamic database of over 1400 species each involving two or more components.

For a particular set of chemical components specified by the user, MINTEQA2 will equilibrate the chemical solution to a specified pH and/or Eh, to the partial pressure of a gas phase and/or to a specified solid phase composition. If solids are specified, MINTEQA2 will calculate the concentrations of metals adsorbed via any of seven different adsorption sub-models. Finally, MINTEQA2 will calculate the relative equilibrium saturation indices of solid species and deplete the total dissolved concentration of components via precipitation of over-saturated solids.

MINTEQA2 is accompanied by an interactive program, PRODEFA2, which is used to create MINTEQA2 input files. In addition to accessing the currently available reaction species from the MINTEQA2 database, PRODEFA2 is capable of defining other aqueous, solid, or adsorption reaction species not currently in the thermodynamic database.

Data Needs

In general, the data needed to run MINTEQA2 consist of a chemical analysis of the sample to be modeled giving total dissolved concentrations for the components of interest. A measured value for pH may be used as an equilibrium pH or an initial guess at equilibrium pH depending on the state of the sample with respect to equilibrium. Eh measurements, while generally unreliable, may be treated in a manner similar to pH. If appropriate, a measured amount of a mineral may be specified as initially present but subject to dissolution if equilibrium conditions warrant. The user must supply equilibrium constants for all adsorption reactions.

Experience

MINTEQA2 may be used for both surface water and ground water problems where speciation and mobility are of concern. Some applications of this or predecessor models [41] include modeling the mobility of copper leaching from mine tailings, modeling the sorbed/solid phase vs. dissolved phase concentrations of Zn, Pb, Ni, Cu, Cd and other metals in laboratory experiments on leachate samples, determining the worst case pH/Eh combination for metal mobility in ground and surface waters, determining the toxic (free ion) concentration resulting from ingestion of lead contaminated soil, and modeling the concentration of metals from leaching of ash piles.

The model can be used successfully by persons possessing a scientific or engineering background with some exposure to inorganic chemistry (one year of introductory college chemistry). Additional exposure to thermodynamics is helpful.

FOOD AND GILL EXCHANGE OF TOXIC SUBSTANCES

FGETS [42], [43] is a toxicokinetic model that simulates the bioaccumulation of nonpolar organic chemicals by fish from both water and tainted food. Both of these routes of exchange are modeled as diffusion processes that depend upon physico-chemical properties of the pollutant and morphological/physiological characteristics of the fish. FGETS contains a moderately sized database of allometric relationships for gill morphology with which it can simulate the direct gill/water exchange of organic chemicals for essentially any fish species, assuming certain default values. FGETS also contains a limited database of physiological/morphological relationships that are used to parameterize food exchange. In addition to simulating bioaccumulation of organic toxicants, FGETS also can calculate time to death from chemicals whose mode of action is narcosis. This calcula-

tion is based on the existence of a single, lethal, internal chemical activity for such chemicals.

The concentrations of toxic chemical to which the food chain is exposed may be specified by the user or may be taken directly from the values calculated by the exposure concentration model WASP4. Thus FGETS may be executed as a separate model or as a post-processor to WASP4.

Variables and Processes

FGETS predicts temporal dynamics of a fish's whole body concentration of a nonmetabolized organic chemical. The chemical is bioaccumulated either from water only, which is, perhaps, the predominant route of exchange during acute exposures, or from water and food jointly, which is the more characteristic route for chronic exposures. These dynamics are calculated algebraically as the ratio of the fish's predicted total body burden to its live weight. The dynamics are simulated by a system of coupled differential equations.

Fish growth is modeled using a mass balance equation accounting for feeding fluxes, egestive fluxes, respiratory fluxes, and its dynamic action. The total body burden is modeled using a mass balance equation accounting for the fish's total gill area, the chemical's mass conductance through the interlamellar water of the gills, the chemical's concentration in the environmental water and in the aqueous blood, and the net mass exchange across the fish's intestine from food.

The gill exchange is simply a direct application of Fick's first law of diffusion. FGETS allows a user to select one of three possible model formulations to represent chemical exchange from food. This exchange can be modeled assuming either a constant toxicant assimilation efficiency, in which the fish's feces and whole body are thermodynamically equilibrated, or a kinetic expression of Fick's first law of diffusion.

The relationship between a chemical's concentration in whole fish and its aqueous fraction is treated conceptually as if the fish were a three-phase solvent consisting of water, lipid, and structural organic matter. It is assumed that equilibration among these phases is rapid in comparison to exchange across the fish's gills and intestine. Consequently, a fish's whole body concentration can be related to its aqueous concentration by the sum of its aqueous fraction, its lipid fraction times the partition coefficient between lipid and water, and its structural organic fraction times the partition coefficient between structural organic matter and water.

Data Needs

To use FGETS, a user must specify several input parameters:

1. the scientific name of the fish, its family, and its life form, i.e., freshwater or marine,
2. the chemical molecular weight, molar volume, melting point, and log octanol-water partition coefficient,
3. the fish's initial live weight,
4. the fish's lipid content as a proportion of its total body weight,
5. the fish's initial whole body concentration of the chemical,
6. an exposure scenario, i.e., the chemical's aqueous concentration as well as the prey concentration over time.

The fish's species name, family, and life form are used to assign the gill morphometric parameters using the model's data file containing allometric functions for gill parameters. Extrapolations are made from data on other fish in the same genus, family, or life form if necessary. The name, family, and life form also are used to assign the physiological parameters such as feeding and respiration rates and assimilation efficiencies that are provided in the model's physiological data base.

The user must specify an adjustment factor representing the active gill area, or the ratio of its physiological to anatomical surface area. This calibration factor is generally between 0.33 and 1.00.

The chemical's aqueous environmental concentration can be input as either an arbitrary time series (generated by the user or by a specified WASP4 simulation), or as a constant, sinusoidal, or exponential function of exposure time. Chemical concentrations in the prey are assumed to be a fixed proportion of that predicted by thermodynamic equilibrium. This proportion can be either less than or greater than unity to account for biomagnification of prey.

Output of the Assessment

FGETS provides a time series of whole fish concentrations, a cumulative frequency plot, the average whole fish concentration, and the effective bioaccumulation factor.

Limitations

FGETS is limited to nonpolar organic chemicals that are not metabolized by fish. Ionizable chemicals may be treated using careful external calculations by the user. As of winter 1989, the morphological data base contained 32 species. The physiological data base contained data on brown trout, rainbow trout, lake trout, arctic char, walleye, and sauger.

Experience

FGETS has been preliminarily validated and appears capable of predicting dynamic internal body concentrations of organic chemicals in fish. It can be used for rapid screening of exposure scenarios for those fish in its data base. Although little expertise is necessary to obtain screening results for these fish, knowledge and experience will greatly help in any site-specific applications.

WASP FOOD CHAIN MODEL

The WASP Food Chain Model (FCM2) is a generalized model of the uptake and elimination of toxic chemicals by aquatic organisms [44]. It is a mass balance calculation in which the rates of uptake and elimination are related to the bioenergetic parameters of the species. A linear food chain or a food web may be specified. Concentrations are calculated as a function of time and age for each species included. Exposure to the toxic chemical in food is based on a consumption rate and predator-prey relationships that are specified as a function of age. Exposure to the toxic chemical in water is functionally related to the respiration rate. Steady state concentrations also may be calculated.

The concentrations of toxic chemical to which the food chain is exposed may be specified by the user or may be taken directly from the values calculated by the exposure concentration model WASP4. Thus FCM2 may be executed as a separate model or as a post-processor to WASP4. Migratory species, as well as non-migratory species, may be considered. Separate non-migratory food chains may be specified and the migratory species is exposed sequentially to each based on its seasonal movements.

Variables and Processes

The concentration of a toxic substance that is observed in an aquatic organism is the result of several uptake and loss processes that include transfer across the gills, surface sorption, ingestion of contaminated food, desorption, metabolism, excretion, and growth. These processes are controlled by the bioenergetics of the organism and the chemical and

physical characteristics of the toxic substance. For phytoplankton and detrital organic material representative of the base of the food chain, sorption-desorption controls toxic substance accumulation. Because the sorption rates are generally much faster than the uptake and excretion rates of species at higher levels of the food chain and the transport and transformation rates of the toxic substance, instantaneous equilibrium is assumed.

For species above the phytoplankton/detritus level, uptake of toxicant due to ingestion of contaminated food is considered. This uptake depends upon the toxicant concentration in the food, the rate of consumption of food, and the degree to which the ingested toxicant in the food is actually assimilated into the tissues. The rate of consumption of food is dependent on metabolic requirements and the growth rate.

The uptake of toxicant from water is determined by the rate of transfer of toxicant across the gills. This rate of transfer is calculated from the rate of transfer of oxygen from water to the blood of the fish, adjusted by the relative diffusivity of the chemical to that of oxygen.

The rate of loss of the toxicant from an organism is the sum of the excretion and detoxification or degradation rates of the chemical. If the organism is exposed to the toxicant in water only, this rate is related to the uptake rate by the bioconcentration factor. The loss rate incorporates several excretory processes, including renal and hepatic excretion, diffusion from blood across the gill, and diffusion from blood across the gut wall. This use of a single rate effectively lumps parameters from more fundamental processes in an empirical manner. In the model, the excretion rate may be internally calculated from a specified bioconcentration factor, or it may be specified directly.

Data Needs

Use of the model requires the determination of an appropriate food chain for the natural water system being considered, and the specification of a number of bioenergetic and toxic chemical related parameters for each member of the food chain. In general the top component of the food chain is chosen first. The feeding habits of this species define additional species whose feeding habits, in turn, define still further species until the base of the food chain is reached. A single species often may be used as representative of a class of species at a given trophic level.

The specific parameters required for each species in the model include bioenergetic related parameters -- growth rate, respiration rate, assimilation efficiency of food, and predator-prey relationships -- and toxic

chemical related parameters -- assimilation efficiency of chemical in food, molecular diffusivity of the toxicant, and bioconcentration factor or whole body excretion rate.

Output of the Assessment

FCM2 calculates time variable concentrations of toxicant in the bodies of plankton and fish comprising food chains in spatially averaged compartments. Concentrations are calculated as a function of time and age class for each species included. Both migratory and non-migratory species can be simulated.

Limitations

FCM2 bases its calculations on empirically derived parameters that effectively lump parameters from more fundamental processes. The relative importance of these underlying processes will vary depending on the metabolic rate of the animal, the route of exposure to the chemical, and the characteristics of the chemical. Care must be taken in properly calibrating this model to site-specific data, and extrapolations should be limited or carefully qualified.

Experience

This model may be applied to any type of natural water system. It has been successfully used to model PCB in the Lake Michigan lake trout food chain [45], PCB in Lake Huron yellow perch food chain, and kepone in the James River striped bass food chain [46]. Applying FCM2 requires both modeling sophistication and biological judgment.

SUMMARY

This paper has reviewed 12 simulation models available from EPA's Center for Exposure Assessment Modeling. The software is completely in the public domain and source code is provided with the programs. Users are encouraged to register with the CEAM in order to receive continuing information on software updates and training opportunities.

ACKNOWLEDGEMENTS

This paper has been largely compiled from abstracts prepared by the various model developers. As such, the authors acted more in the capacity of editors than writers and are indebted to the model developers for supplying much original material.

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